

Impurity Effect on Ferromagnetic Transition in Double-Exchange Systems

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Abstract

Effect of randomness in the double-exchange model is studied. Large fluctuations and spatial random distribution of impurities are taken into account in an essentially exact manner by using the Monte Carlo calculation. The randomness suppresses the ferromagnetism by reducing the coherence of itinerant electrons. The suppression is significant in the critical region where the fluctuations are dominant. Temperature dependences of the magnetization are estimated for finite-size clusters. A characteristic temperature for phase transition T^* is estimated from the inflection point, which is expected to give a good approximation for the critical temperature in the thermodynamic limit. Our results suggest that the ferromagnetism becomes unstable more rapidly than predicted in the previous theoretical results by the coherent-potential approximation.

Key words: D. magnetic properties, D. phase transitions, A. magnetic materials

1 Introduction

The double-exchange (DE) model has been studied intensively to explain ferromagnetic transition in colossal-magnetoresistance manganites. [1] The origin of the metallic ferromagnetism in these materials is well explained by the DE mechanism. [2] Recently, numerical calculations have demonstrated that fluctuations through the strong interplay between spin and charge degrees of freedom play a crucial role in this system. [3–6] Through precise calculations

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of the ferromagnetic transition temperature T_c , the DE model is shown to give a quantitative description of the ferromagnetic transition in the typical material $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ near $x = 0.3$. This provides a well-established starting point toward comprehensive understanding of rich variety of physics in the manganites through quantitative comparisons between experiments and theories.

To this canonical DE ferromagnetic state, there are various perturbations in experiments, for instance, control of chemical compositions, external pressure and magnetic field. [7] It is important to clarify these effects theoretically in order to understand experiments where the perturbations may be entangled and act on in a complicated manner. Among them, we study effects of the randomness in this paper. Since mixed-valence manganites are synthesized as solid solutions, randomness is inevitably contained in these compounds. We discuss how the ferromagnetic transition is affected by the randomness.

The randomness effect for T_c in the DE system has been studied theoretically. Stability of the ferromagnetic state is studied by the coherent-potential approximation (CPA), and a decrease of T_c due to the randomness is predicted. [8–10] In this work, we go beyond the approximation and use a numerical technique which is essentially exact. Spatial random distribution of impurities is taken into account properly in this method. Since the spatial fluctuations which are neglected in the CPA are known to be important in the case without disorder, [3] the unbiased calculations are necessary also for the systems with disorder to discuss the quantitative change of T_c .

This paper is organized as follows. The next section 2 introduces the DE model with disorder and describes the numerical methods briefly. In Sec. 3, the results for the approximately-estimated critical temperature are discussed for the cases with randomness in comparison with the results for the pure system. Sec. 4 is devoted to summary and concluding remarks.

2 Model and Method

In this work, we consider a simple model with a diagonal disorder in the framework of the DE model. The Hamiltonian is explicitly given by

$$H = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - J_H \sum_i \vec{\sigma}_i \cdot \vec{S}_i + \sum_{i\sigma} \varepsilon_i c_{i\sigma}^\dagger c_{i\sigma}, \quad (1)$$

where the first term denotes the nearest-neighbor hopping on the cubic lattice and the second term is for the Hund's-rule coupling. The last term denotes the on-site randomness which modifies the one-body potential energy in each

site. The potential ε_i takes $\pm W_{\text{imp}}/2$ in equal probability in each site. The physical quantities are calculated by the random average for the quenched disorder. For simplicity, we consider the limits of $J_H \rightarrow \infty$ and $|\vec{S}| \rightarrow \infty$. In the following, we discuss the quarter-filled case which shows a maximum of T_c in the pure case.

We apply the Monte Carlo (MC) method to the model (1). [11–13] In this method, the MC weight to update a configuration of the localized moments are calculated quantum-mechanically by integrating out the fermion degrees of freedom. For large-size clusters, the difficulty of a rapid increase of the computational time has been solved by using the moment-expansion MC method. [12,13] The moment expansion as well as the random average is performed quite efficiently on parallel computer systems.

In the following, we use an energy unit $W = 6t = 1$ which is the half bandwidth for the pure system. For a given configuration of disorder, we have typically run 1,000 MC samplings for measurements after 1,000 MC steps for thermalization. The random average is taken for 50 random configurations.

3 Results and Discussions

Before going to the cases with randomness, we review and discuss the ferromagnetic transition in the pure case ($W_{\text{imp}} = 0$). [3] Figure 1 shows the results for the temperature dependence of the magnetization for $W_{\text{imp}} = 0$. We present the data for finite-size clusters and those for the thermodynamic limit. The latter is obtained by the finite-size scaling analysis. From the onset of the magnetization in the thermodynamic limit, T_c is estimated as $T_c/W = 0.023 \pm 0.003$.

Figure 1 indicates that in order to obtain the precise estimate of T_c , a systematic study of the finite-size effects is crucial, which needs much computational effort. We note, however, that it is possible to define a characteristic temperature even for a fixed-size cluster. The temperature dependence of the magnetization for each finite-size cluster is a monotonic function and has an inflection point. We adopt this inflection point as the characteristic temperature T^* . In Fig. 2, we plot the system-size dependence of T^* which is obtained from the numerical differentiation of the data in Fig. 1. Within the error bars, T^* is almost independent of the system size and agrees with T_c in the thermodynamic limit. Thus, T^* for a finite-size cluster is expected to give a good approximation for T_c in this pure case. We expect that this observation holds also for the systems with randomness below. Note that at least, since T^* must be an independent parameter to characterize the temperature scale for the ferromagnetic transition, it should be justified to discuss the stability of the ferromagnetism by T^* .

Now we discuss the randomness effect. Figure 3 shows the magnetization curve for the system size of $4 \times 4 \times 4$ sites when we change the value of W_{imp} . The magnetization decreases as the disorder strength W_{imp} increases. This indicates that the ferromagnetism is suppressed by the randomness. The decrease is the most significant near $T_c(W_{\text{imp}} = 0)$. This is probably because near the critical point, the fluctuations are dominant and the coherence of the itinerant electrons becomes very sensitive to the randomness.

Based on the discussion in the pure case, we examine the stability of the ferromagnetism in the systems with randomness by T^* . Figure 4 shows T^* as a function of W_{imp} which is estimated from the data in Fig. 3. As the critical temperature in the previous CPA results, [8–10] the approximated critical temperature T^* decreases as W_{imp} increases. Our MC data, however, show larger decrease in comparison with the CPA results: For instance, for $W_{\text{imp}}/W = 0.5$, our data show about 35% decrease, while the CPA results show less than 20% decrease. The CPA takes account of the randomness in an averaged way through the change of the density of states. In our MC study, the spatial distribution of the randomness as well as its effect on the coherence of electrons is included properly. Our data suggest that the spatial fluctuations are important and the suppression of T_c is stronger than expected from the band renormalization in the CPA.

4 Summary and Concluding Remarks

We have investigated the randomness effect on the ferromagnetic transition in the double-exchange model. We consider the model with on-site diagonal disorder. The spatial distribution of the randomness and large fluctuations inherent in this strongly-correlated system are taken into account properly by using the Monte Carlo method. The randomness suppresses the ferromagnetism of the double-exchange origin by reducing the coherence of the electron motion. Our results indicate that the suppression is significant in the critical region where the fluctuations are dominant. We have examined the characteristic temperature scale which is expected to give a good approximation for the critical temperature. The approximated critical temperature tends to be suppressed by the randomness as predicted by the coherent-potential approximation. Our Monte Carlo results, however, show a more rapid decrease than the previous results. This may be attributed to the spatial fluctuations by the randomness distribution which is included only in an averaged manner in the previous approximations.

The randomness effects are studied only for a small-size cluster in this paper. The estimated temperature T^* is an approximation for T_c . Calculations for larger-size systems and more precise determination of the critical temperature

including the finite-size scaling are under investigation. Different distribution of the randomness is also examined and will be reported elsewhere.

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References

- [1] N. Furukawa: *Physics of Manganites*, eds. T. Kaplan and S. Mahanti (Plenum Publishing, New York, 1999), and references therein.
- [2] C. Zener, Phys. Rev. **82** (1951) 403.
- [3] Y. Motome, N. Furukawa, J. Phys. Soc. Jpn. **69** (2000) 3785; *ibid.* **70** (2001) No.10 in press.
- [4] Y. Motome, N. Furukawa, J. Phys. Soc. Jpn. **70** (2001) 1487.
- [5] Y. Motome, N. Furukawa, J. Phys. Soc. Jpn. **70** (2001) 2802.
- [6] N. Furukawa, Y. Motome, cond-mat/0107172.
- [7] A. P. Ramirez, J. Phys.: Condens. Matter **9** (1997) 8171, and references therein.
- [8] B. M. Letfulov, J. K. Freericks, cond-mat/0103471.
- [9] M. Auslender, E. Kogan, cond-mat/0105550.
- [10] M. Auslender, E. Kogan, cond-mat/0106032.
- [11] S. Yunoki, J. Hu, A. Malvezzi, A. Moreo, N. Furukawa, E. Dagotto, Phys. Rev. Lett. **80** (1998) 845.
- [12] Y. Motome, N. Furukawa, J. Phys. Soc. Jpn. **68** (1999) 3853.
- [13] N. Furukawa, Y. Motome, H. Nakata, cond-mat/0103316.

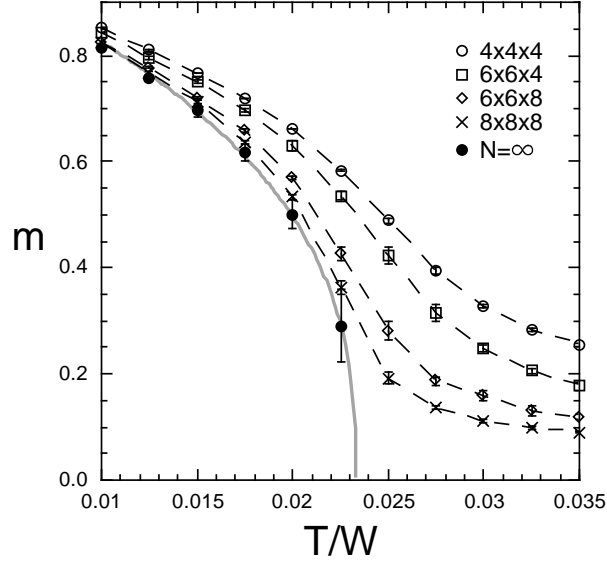


Fig. 1. Temperature dependence of the magnetization for the pure system. The dashed lines connecting the data for finite-size clusters are guides for the eye. The gray curve for the data in the thermodynamic limit is a scaling fit of $m \sim (T_c - T)^\beta$.

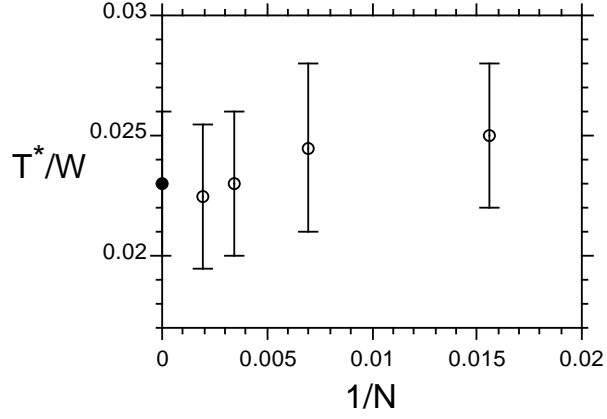


Fig. 2. System-size dependence of the temperature of the inflection points in the magnetization curve for the finite-size clusters. The data on the vertical axis is the estimate of T_c in the thermodynamic limit.

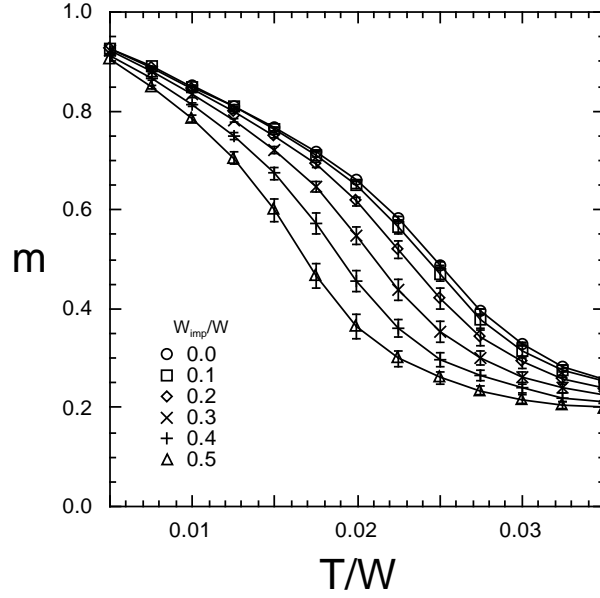


Fig. 3. Temperature dependence of the magnetization for the systems with randomness. The data are for the cluster with $4 \times 4 \times 4$ sites. The lines are guides for the eye.

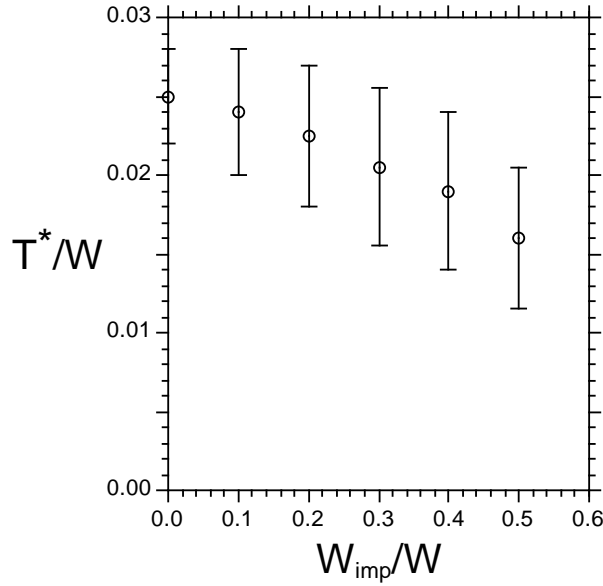


Fig. 4. The approximately-estimated transition temperature as a function of the strength of the randomness. The data are estimated from the inflection points in the magnetization curve in Fig. 3.